# netlognews

*NETL's R&D newsletter* *July 2010, Issue 18*

## $CO_2$ Tracer Technology Successfully Tested

page 2

## High Speed Particle Imaging Shows Success

page 3

## $CO_2$ Reuse Photocatalysts One of Top 10 Most Accessed Papers

page 5

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## CONTENTS



### ON THE COVER

*NETL technician Hank Rush connects plumbing to inject tracer at the Lower Michigan Basin sequestration site.*

Netlognews is a quarterly newsletter, highlighting recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.

*NETL technician Hank Rush connects plumbing to inject tracer at the Lower Michigan Basin sequestration site.*

## $CO_2$ Tracer Technology Successfully Tested

The ability to detect and track the movement of carbon dioxide ($CO_2$) in underground geologic storage reservoirs—an important component of carbon capture and storage (CCS) technology— has been successfully demonstrated at a U.S. Department of Energy (DOE) San Juan Basin coalbed test site in New Mexico.

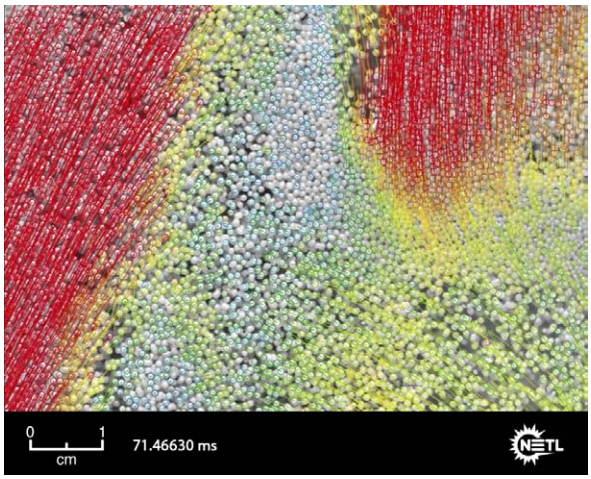
NETL's SEQURE™ tracer technology uses perfluorocarbon tracers (PFTs)—non-toxic, chemically inert, clear colorless liquids—to provide a verifiable way to measure $CO_2$ movement as well as providing leak detection.

Demonstrating and confirming long-term $CO_2$ storage security is an important precondition to large-scale deployment of carbon capture and storage, a significant part of a portfolio approach to help meet the challenge of global climate change.

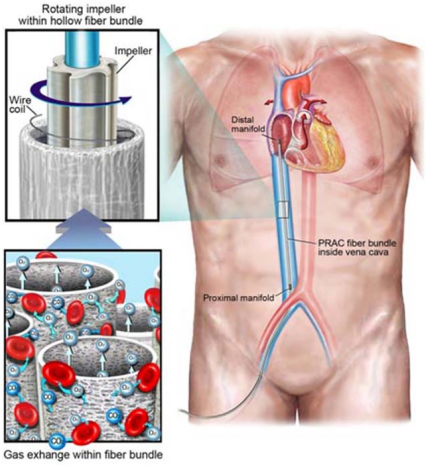
In 2009, the patent-pending SEQURE technology earned *R&D Magazine's* prestigious R&D 100 Award, emblematic of one of the top 100 most significant products introduced to the marketplace during the past year.

For the full story, click here.

Contact: Rodney Diehl, 412-386-6146




*The HSPI system measures the velocity of fluids and can accurately recognize and measure particle motion inside particle flows.*




*NETL's high-speed particle imaging system accurately images human blood flow, which closely resembles the high concentration particle flow of fossil energy processes. Image courtesy of the Medical Devices Laboratory--McGowan Institute*

## High Speed Particle Imaging Shows Success

Imagine following a particle smaller than a grain of salt among millions of particles moving randomly in a high-speed liquid or gas stream. High-concentration particle flows are not only microscopic, they are opaque, and their high speed has made them difficult to study.

Although high concentration particle flow is critically important to many chemical, energy, biological, and food processes, until recently researchers could not see how particles moved within them. In fossil energy processes, high-concentration particle flow fields (HCPFFs) are important in situations such as fluidized beds, pulverized coal combustion, advanced gasification, $CO_2$ capture and sequestration, and gas stream clean-up.

Computational fluid dynamics (CFD) models of HCPFFs can be used to design and optimize new fossil energy systems. Until recently, modelers had not been able to see what they were modeling. This makes it difficult to know if their models are accurate.

A new high-speed particle imaging velocimetry (HSPIV) system now provides the first detailed view of particle motion and the first accurate measurements inside HCPFFs. Over the past two years, the first software has been developed that can accurately recognize and measure particle motion inside these fields. A patent application for the HSPIV software has been filed with the U.S. Patent Office, and discussions are underway with private sector companies who may be interested in licensing the technology.

The HSPIV system is currently being used at a chemical/energy industry research lab in Chicago (PSRI), and at the McGowan Institute for Regenerative Medicine in Pittsburgh in another application--to study blood flow in a respiratory assist catheter.

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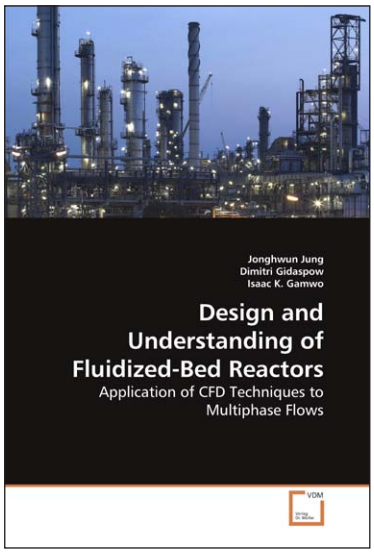


## Applying CFD Techniques to Fluidized-bed Reactors Book Published

"Design and Understanding of Fluidized-Bed Reactors: Application of CFD Techniques to Multiphase Flows," authored by Jonghwun Jung, Dimitri Gidaspow, and Isaac K. Gamwo, was recently published by VDM Verlag. The book is a spinoff of the doctoral research of Dr. Jung, which was conducted at NETL. The authors were contacted by Verlag about publishing the research as a book due to its practical relevance and the high demand for Dr. Jung's dissertation from various research institutions throughout the world.

The book describes practical applications of multiphase computational fluid dynamics (CFD) models with the kinetic theory of granular flows in bubbling, turbulent, and fluidized-bed reactors. It explains bubble behaviors, hydrodynamics, and reaction kinetics for scaling up such reactors using two multiphase CFD codes. The book is useful to research engineers working on fluidization technology and researchers studying multiphase flows, computational fluid dynamics, and fluidization.

Dr. Gamwo of NETL and Professor Gidaspow of IIT (Chicago) supervised Dr. Jung's Ph.D. research work at NETL. The two multiphase CFD codes referred to are the IIT code and the MFIX code. The latter was developed at NETL. The book also discusses two kinds of granular temperatures that affect solid diffusions and mixing in particle and bubble levels, as well as a technique to optimize catalyst size in fluidized catalytic reactors.

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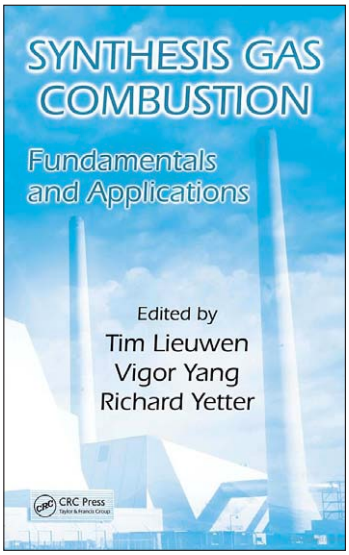


## NETL Researchers Contribute to New Syngas Combustion Book

Because of its potential role in future electric power generation, there is increased interest in the use of coal- and bio-derived synthesis gas, or syngas. To address this interest, CRC Press/Taylor & Francis recently published a compilation of research in this area titled, "Synthesis Gas Combustion: Fundamentals and Applications." NETL researchers contributed chapters on "Gasification Technology to Produce Synthesis Gas" and "Syngas Utilization." The first chapter reviews the background and history of gasification processes and implications of the different gasification technologies. The utilization chapter explains tradeoff issues and R&D issues associated with using syngas in different application areas such as fuels, chemicals, electrical production, $CO_2$ removal, and management. These chapters have already been cited in several technical publications.

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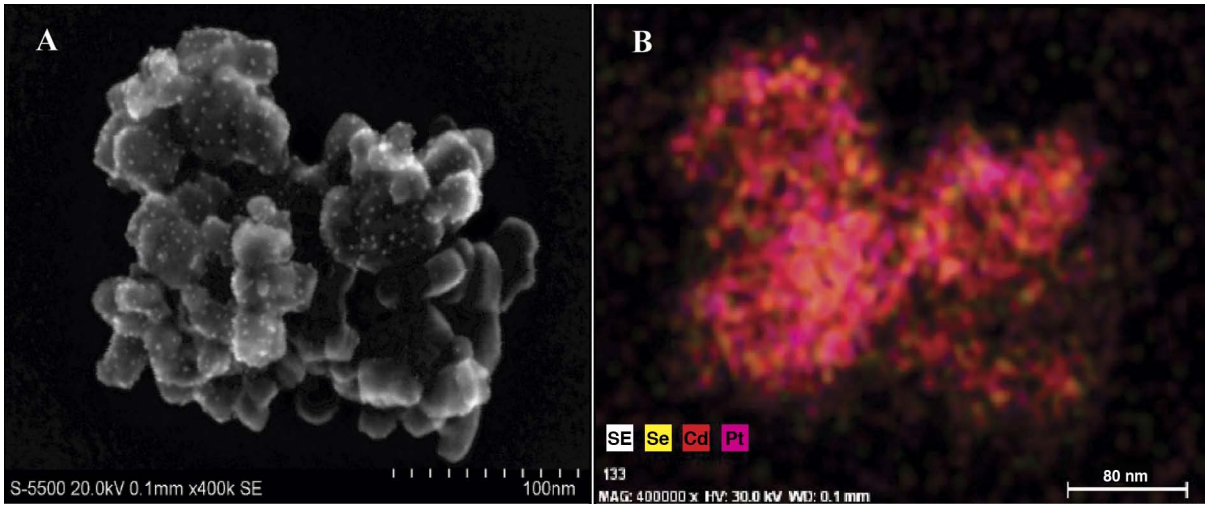


*(A) SEM image of the new photocatalyst, 100 nanometers, and (B) EDS mapping of the same sample, 80 nanometers.*

## $CO_2$ Reuse Photocatalysts One of Top 10 Most Accessed Papers

The *Journal of Physical Chemistry Letters*, published by the American Chemical Society, recently announced that an NETL publication titled "Visible Light Photo reduction of $CO_2$ Using CdSe/Pt/$TiO_2$ Heterostructured Catalysts" was one of the top 10 most accessed journal articles in 2010. This distinction illustrates the scientific community's interest in development of new $CO_2$ management technologies.

The paper describes the synthesis and characterization of a new photocatalyst, as well as its ability to convert $CO_2$ into value-added fuels and chemicals such as methanol and methane. Previous photocatalysts for this application were activated by ultraviolet light, which makes up only 1–5% of the light reaching the Earth's surface. The new catalyst is activated by visible light, which is the majority of the sunlight that reaches us. Visible light activation makes the catalytic process more efficient--an advance of paramount importance for $CO_2$ reuse applications. The catalyst activity can be systematically tuned to use different colors of visible light by controlling the size of the semiconductor nanocrystals that make up the catalyst.

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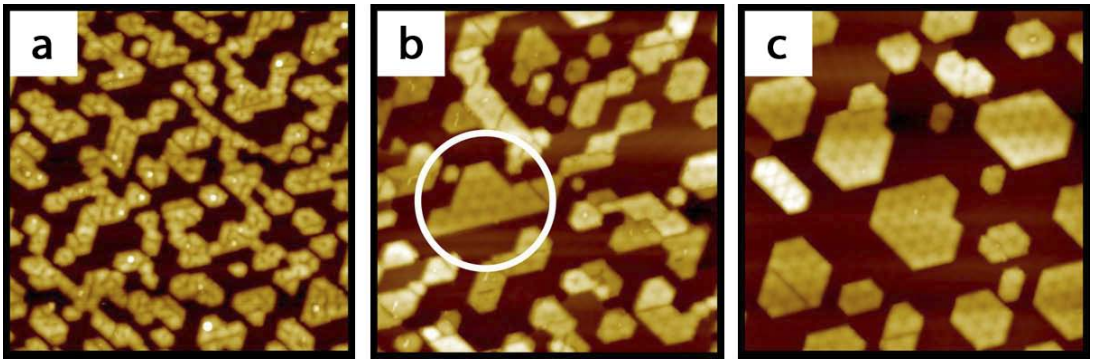


*Room temperature scanning tunneling microscope images of (a) 1 MLE a-$Fe_2O_3$ on Au(1 1 1) (I = 25 pA, V = 1.2 V), and after annealing in UHV at 750 K for (b) 10 min (I = 50 pA, V = 1.0 V) and (c) 30 min (I = 50 pA, V = 1.0 V). Image sizes are 100 X 100 $nm^2$.*

## New Insight into Activating Fischer-Tropsch Catalysts

The Fischer–Tropsch (F-T) process is a set of chemical reactions that historically has been used to produce a petroleum substitute from coal, natural gas, or biomass by nations looking for an alternative to importing it. The F-T process has received intermittent attention as a source of low-sulfur diesel fuel whenever the cost of petroleum gets sufficiently high. It can also be used to create hydrogen from the same raw materials, which makes it interesting to researchers who are developing new technologies for cheaper ways to power a fuel cell.

Catalysts are a key component of the F-T process. A common catalyst is iron oxide, $Fe_2O_3$ (commonly referred to as rust), which is transformed into $Fe_3O_4$, FeO, Fe, and Fe-carbides during the F-T process. The arrangement of the surface atoms on the iron compounds dictates how reactive these catalysts are. Although F-T catalysts have been in use for several decades, there are no experimental data on how the arrangement of atoms on the surface of these catalysts evolves during the F-T process.

Researchers at NETL recently used a scanning tunneling microscope to image how the arrangement of surface atoms on these catalysts evolves during the F-T process. This specialized instrument allowed researchers to directly "see" individual atoms on the surface of these catalysts and compare them to computational models that predict what arrangements of atoms should exist. The combined approach of using advanced instrumentation and computational models has shed new light on how these F-T catalysts can transform gasified coal into useful fuels. The results indicate that these catalysts appear to have a tightly packed arrangement of oxygen atoms on their surface and that the more reactive iron atoms reside below this layer of oxygen atoms. This suggests that large facets of the catalyst surface are unreactive towards F-T chemistry and that imperfections in this oxygen arrangement are responsible for the activity of these catalysts. This also seems to indicate that smaller catalyst particles with more defects and particle edges may be more efficient for the F-T process. The journal *Surface Science* recently published this study in vol. 604, pp. 627-632.

Contact: Christopher Matranga, 412-386-4114

## Seismic Surveys Track Carbon Dioxide Movement Underground

Researchers and collaborators at NETL and the University of Pittsburgh have developed a correlation between acoustic wave velocity and relative $CO_2$ saturation to calibrate and refine the interpretation of 3D seismic reflection surveys.

Discussed in a special section on $CO_2$ sequestration in *The Leading Edge* (Vol. 29 (2010), No. 2, pg. 192ff.), the lab-scale study conducted with actual reservoir rocks shows the procedure could be employed to effectively track the movements of $CO_2$ after injection for carbon sequestration or enhanced oil recovery.

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## Coal Seam Carbon Sequestration Successfully Simulated

A newly developed model used to determine the geomechanical responses of coal-seam systems has improved the simulation of coal permeability and agreement with field data obtained from the Allison field in northwest New Mexico—the world's first enhanced coalbed methane/carbon sequestration field project. In addition to permeability, the model yields a better description of the roles of coal shrinkage and swelling, coal elastic properties, cleat porosity, and better estimates for geophysical parameters that are difficult to measure in the laboratory. Results of the study appear in a special section on $CO_2$ sequestration in *The Leading Edge* (Vol. 29 (2010), No.2, pg. 224ff.) published by the Society of Exploration Geophysicists.

Contact: Duane H. Smith, 304-285-4069

*Small scale extinguishing experiments of coal subsurface fires. Illustration courtesy of Hadden, R. and G. Rein*, University of Edinburgh.

## NETL Explores Potential Beneficial Uses of Captured $CO_2$

U.S. coal-burning power plants emit more than 2 billion tons of carbon dioxide ($CO_2$) per year. In anticipation that $CO_2$ capture from these plants will be required in the future, research is underway on capture technology, underground storage of $CO_2$, and enhancing beneficial uses. Current uses for $CO_2$ include fire suppression, food preservation, refrigeration/cooling, beverage carbonation, welding, enhanced oil recovery, coalbed methane recovery, supercritical cleaning, biomass production, and polymer-plastic manufacture.

The lab is conducting research on incorporating captured $CO_2$ in plastics manufacture; combined coal mine fire suppression and gasification; catalytic synthesis of fuels (i.e., methane and methanol); and production of synthetic fuels from algae.

An unusual potential application is suppression of fires in underground mines. Underground coal fires are notoriously difficult to extinguish, responsible for as much as 3% of the world's annual $CO_2$ emissions, and consume as much as 5% of its mineable coal.

Some issues in the beneficial use of $CO_2$ captured from power plants include the location of the power plant and utilization project, the distribution and transport of the $CO_2$, and the purity required for the $CO_2$ application.

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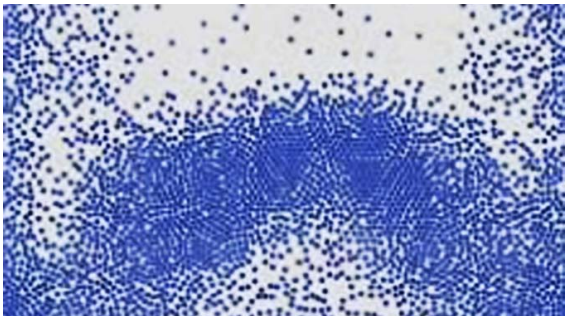

## NETL Initiates the World's Most Comprehensive Benchmarking of Fluid Dynamic Models

NETL and Particulate Solid Research Inc. (PSRI) have prepared the 3rd Computational Fluid Dynamics (CFD) Challenge Problem Package, which was presented to the international commercial and academic CFD community at the NETL MFIX website on May 9, 2010. MFIX is a general purpose computer code developed by NETL researchers used to describe the hydrodynamics, heat transfer, and chemical reactions in fluid-solids systems.

The challenge being presented is to model the behavior of selected bed materials in the NETL circulating fluidized bed and the PSRI bubbling fluid bed. Model predictions will be compared against actual experimental results and the results of those comparisons will be presented at the Circulating Fluid Bed X to be held in Sun River Valley, Oregon in May 2011. Modelers have been given detailed descriptions of the NETL and PSRI experimental facilities as well as information on the four different bed materials being tested. By comparing the predicted behavior with behavior actually experienced, strengths and weaknesses associated with the different modeling approaches will be identified and shortcomings can be targeted for future development and improvements.

To ensure that poor validation results do not result from incomplete information supplied to the modelers, the Challenge Problem developers have instituted a multistep process. After submission of the first modeling results, each participant will be given the opportunity to refine model predictions using actual experimental data, which will be made available November 1, 2010. Modelers will then be allowed to resubmit their refined model results. Both the results from the initial and refined models will be published with explanations for any discrepancies.

At the conclusion of the challenge problem, the problem statement and associated data will be available for years to come giving model developers a 'tested' set of validation data.

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## NETL and CMU Launch Collaborative Initiative

NETL researchers, faculty at Carnegie Mellon University (CMU), and industrial participants in CMU's Center for Advanced Process Decision-making (CAPD) launched an Energy Systems Initiative (ESI) to collaborate in developing energy-efficient and sustainable processes. The ESI allows NETL and CMU to expand current process and dynamic systems research efforts with industry-centered projects conducted within a special interested group composed of researchers and practitioners. The ESI collaboration establishes a broader research base in the energy area by jointly exploring new funding initiatives. NETL and CMU launched the ESI with a successful one-day kickoff meeting attended by more than 30 CAPD members from CMU, NETL, and industry, including Air Products and Chemical, Dow Chemical, Eastman Chemical, Ecopetrol, Exxon Mobil, NOVA Chemicals, Petrobras, PPG Industries, and Praxair.

With support from DOE, the National Science Foundation, member organizations, and other funding agencies, the CAPD research center (http://capd.cheme.cmu.edu/) has pioneered the discovery, development, and application of new methods for process design, analysis, and operations. The NETL Collaboratory for Process & Dynamic Systems Research—organized among NETL, CMU, the Pennsylvania State University, the University of Pittsburgh, Virginia Tech, and West Virginia University—is a member of CAPD and addresses process systems engineering challenges arising across the energy power plant lifecycle.

Contact: David C. Miller, 304-285-6550

## Fuel Cell/Turbine Hybrid System Successfully Simulated

A recently completed preliminary study demonstrated the first hardware simulation of a fuel cell/turbine hybrid with a distributed fuel cell model capable of operating in real-time. The study described the system level impact of fuel cell load changes and described fuel cell temperature profiles, species concentration gradients, and current density variations over the fuel cell length.

Significant current density variations were observed at the fuel cell inlet, while sequential temperature variations were greatest at the fuel cell outlet. The peak temperature gradient increased by 40%. Fuel cell diffusion losses were greatly impacted during a load transition, changing by as much as 20% over a 3-second period. Quantifying these expected gradients is essential to specifying stack geometry design and cathode flow control actuator requirements for the fuel cell system in a hybrid.

This study provided the international hybrids research community with a glimpse of distributed fuel cell performance during coupled transient operation and employed the unique capability of the NETL Hyper (hybrid performance) facility. The Hyper facility provides a unique opportunity for researchers to explore issues related to the coupling of fuel cell and gas turbine technologies.

This research was recently presented at the 2010 International Colloquium on Environmentally Preferred Advanced Power Generation.

Contact: David Tucker, 304-285-4182


## Inspection Sensor for Plastic Pipeline

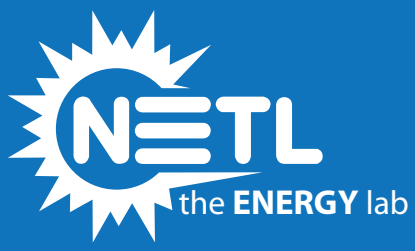
U.S. natural gas transmission and distribution reliability is essential to ensure clean, affordable energy is available to our homes and businesses. Several technologies exist to inspect metal pipelines, but approximately half of the gas distribution pipelines within the United States are made from plastic. The plastic pipeline network is increasing as new capacity is added and aging metal pipes are replaced with polyethylene pipe.

A capacitance sensor technique has been developed that detects changes in the dielectric properties of plastic pipe material. The resulting change in capacitance has been successfully used to identify discontinuities indicating potential trouble spots or a leak point in the pipeline. The sensor development and laboratory test results were presented at the American Gas Association Conference in New Orleans in May and follow-up discussions are now ongoing with interested commercial companies. Our researchers are also looking at other similar needs, such as pre-installation inspection of plastic pipe fusion joints to ensure the integrity of the pipelines before installation.

Contact: Jimmy Thornton, 304-285-4427

# Recent NETL Publications


1. Gamwo, Isaac K. and Yong Lium, "Mathematical Modeling and Numerical Simulation of Methane Production in a Hydrate Reservoir," *Ind. Eng. Chem. Res*., 2010, 49 (11), pp 5231-5245.
2. Lyczkowski, Robert W., Jacques X. Bouillard, Isaac K. Gamwo, Mark R. Torpey, and Eugene D. Montrone, "Experimental and CFD Analyses of Bubble Parameters in a Variable-Thickness Fluidized Bed," Ind. Eng. Chem. Res., 2010 49 (11), pp 5166-5173.
3. Sorescu, Dan C. and Betsy M. Rice, "Theoretical Predictions of Energetic Molecular Crystals at Ambient and Hydrostatic Compression Conditions Using Dispersion Corrections to Conventional Density Functional (DFT-D)," *J. Phys. Chem*. C,2010, 114 (14), pp 6734-6748.
4. Benyahai, Sofiane and Janine E. Galvin, "Estimation of Numerical Errors Related to Some Basic Assumptions in Discrete Particle Methods," *Ind. Eng. Chem. Res*., Article ASAP, 10, 1021/ie100662z, May 3, 2010.
5. Strakey, Peter A., "Development and Validation of a Thickened Flame Modeling Approach for Large Eddy Simulation of Premixed Combustion," *J. Eng. Gas Turbines Power*, July 2010, 132 (7), 071501 (9 pp).
6. Martinez, Andrew, Kirk Gerdes, Randall Gemmen, and James Poston, "Thermodynamic Analysis of Interactions Between Ni-based Solid Oxide Fuel Cells (SOFC) Anodes and Trace Species in a Survey of Coal Syngas," *J. of Power Sources*, 195 (2010) 5206-5212.
7. Shelton, Michael, Ismail Celik, Eric Liese, and David Tucker, "A Study in the Process Modeling of the Startup of Fuel Cell/Gas Turbine Hybrid Systems," *J. Eng. Gas Turbines Power*, Jan 2010, 132 (1) 012301, 8 pp.
8. Xingyi Deng, Junseok Lee, Christopher Matranga, "Preparation and Characterization of $Fe_3O_4$(111) Nanoparticles and Thin Films on Au(111)," *Surface Science*, Elsevier, Volume 604, Issues 7-8 (15 April 2010), pg. 627-632;
9. Wang, Conjung et al., "Visible Light Photoreduction of $CO_2$ Using CdSe/Pt/$TiO_2$ Heterostructured Catalysts," *The Journal of Physical Chemistry Letters*, American Chemical Society, Volume 1 (7 January 2010) No. 1, pg. 48-53.

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